Iterative Solutions for Low Lying Excited States of a Class of Schroedinger Equation*

R. Friedberg[1], T. D. Lee[1, 2] and W. Q. Zhao[2, 3]

1. Physics Department, Columbia University
New York, NY 10027, U.S.A.
2. China Center of Advanced Science and Technology (CCAST/World Lab.)
P.O. Box 8730, Beijing 100080, China
3. Institute of High Energy Physics, Chinese Academy of Sciences
Beijing 100039, China

Abstract

The convergent iterative procedure for solving the groundstate Schroedinger equation is extended to derive the excitation energy and the wave function of the low-lying excited states. The method is applied to the one-dimensional quartic potential problem. The results show that the iterative solution converges rapidly when the coupling g is not too small.

PACS: 11.10.Ef, 03.65.Ge

Key words: iterative solution, low-lying excited state, convergence

---

* This research was supported in part by the U. S. Department of Energy Grant DE-FG02-92ER-40699 and the National Natural Science Foundation of China No.10547001

1. Introduction

Consider the N-dimensional Schroedinger equation

$$(-\frac{1}{2}\nabla^2 + V(q) - E)\psi(q) = 0 \tag{1.1}$$

with

$$q = (q_1,\ q_2,\ \cdots,\ q_N) \tag{1.2}$$

and

$$\nabla^2 = \sum_{i=1}^{N} \frac{\partial^2}{\partial q_i^2}.$$

Through a linear transformation of the coordinates $q_1,\ q_2,\ \cdots,\ q_N$, (1.1) can be applied to most of the nonrelativistic many body problems. Similarly, in the limit $N \to \infty$, the same equation can also be extended to relativistic bosonic field theories. However, except in a few special cases, it is difficult to derive analytical solutions. Recently, for a class of Schroedinger equations we have succeeded in deriving a convergent iterative series solution for the groundstate[1-4]. These include the Sombrero shaped potential in any space dimension and arbitrary angular momentum[5]. In this paper, we discuss possible extension to low lying excited states.

Let

$$\psi_{gd}(q) = e^{-S(q)} \tag{1.3}$$

and E_{gd} be the ground state wave function and the ground state energy. Denote the corresponding ones for the first excited state as

$$\psi_{ex} = e^{-S}\chi \quad \text{and} \quad E = E_{gd} + \epsilon. \tag{1.4}$$

We assume the potential $V(q)$ to have high barriers and low valleys, so that the excitation energy ϵ is very small. As an example, take q to be a one-dimensional space x and

$$V(x) = \frac{g^2}{2}(x^2 - 1)^2 \tag{1.5}$$

with g large. The first excited state would have an excitation energy

$$\epsilon \sim e^{-\frac{4}{3}g} << 1. \tag{1.6}$$

For clarity, we shall also assume that, in the general case of $V(q)$, there is only one such low-lying state, as in the example of the one-dimensional quartic potential.

Let the Schroedinger equations for $\psi_{gd} = e^{-S}$ and $\psi_{ex} = e^{-S}\chi$ be

$$(-\frac{1}{2}\nabla^2 + V - E_{gd})e^{-S} = 0 \tag{1.7}$$

and

$$(-\frac{1}{2}\nabla^2 + V - E_{gd})e^{-S}\chi = \epsilon e^{-S}\chi. \tag{1.8}$$

Multiplying (1.7) by $e^{-S}\chi$ and (1.8) by e^{-S}, we obtain from their difference,

$$-\frac{1}{2}\nabla \cdot (e^{-2S}\nabla\chi) = \epsilon e^{-2S}\chi. \tag{1.9}$$

Replace (1.9) by a series of iterative equations: for $n \geq 1$

$$-\frac{1}{2}\nabla \cdot (e^{-2S}\nabla\chi_n) = \epsilon_n e^{-2S}\chi_{n-1} \tag{1.10}$$

and when $n = 0$,

$$e^{-S}\chi_0 = \text{ a trial function } \psi_{trial} \tag{1.11}$$

which satisfies the orthogonality condition between ψ_{gd} and ψ_{trial}; i.e.

$$\int e^{-2S}\chi_0 d^N q = 0. \tag{1.12}$$

When χ_{n-1} is known, the iteration of (1.10) gives only the ratio χ_n/ϵ_n. To perform the next order iteration it is necessary to separate ϵ_n and χ_n. For this purpose, we may choose a fixed point q^0 and set

$$\chi_n(q^0) = \chi_0(q^0). \tag{1.13}$$

Clearly, different choices of q^0 will yield different sequences of $\chi_n(q)$ and ϵ_n, as we shall discuss.

For given e^{-S} and χ_{n-1}, (1.10) can be viewed as an analog problem in electrostatics with a dielectric constant κ and an external electric charge σ_n given by

$$\kappa = e^{-2S} \quad \text{and} \quad \sigma_n = \epsilon_n e^{-2S}\chi_{n-1} \tag{1.14}$$

Let $\vec{E}_n$ be the corresponding electrostatic field and $\vec{D}_n$ the displacement field. We write

$$\vec{E}_n = -\frac{1}{2}\nabla\chi_n \tag{1.15}$$

and

$$\vec{D}_n = \kappa\vec{E}_n. \tag{1.16}$$

Thus, (1.10) becomes

$$\nabla\cdot\vec{D}_n = \sigma_n. \tag{1.17}$$

At ∞, $\psi_{gd} = e^{-S} = 0$. Therefore $\kappa(\infty) = 0,\ \sigma_n(\infty) = 0$ and

$$\vec{D}_n(\infty) = 0. \tag{1.18}$$

Integrating (1.17) over all space we find, on account of (1.18),

$$\int \sigma_n d^N q = \int e^{-2S}\chi_n d^N q = 0. \tag{1.19}$$

Hence, the orthogonality condition (1.12) is now carried over to all $n \geq 1$.

Expand $e^{-S}\chi_n$ in terms of the set of all eigenstates $\{\psi_a\}$ of (1.1). We have, because of (1.19),

$$e^{-S}\chi_n = \sum_{a\neq gd} c_a(n)\psi_a \tag{1.20}$$

with

$$c_a(n) = \frac{1}{E_a - E_{gd}}\epsilon_n\cdot c_a(n-1). \tag{1.21}$$

For problems like the one-dimensional quartic potential (1.5), when the coupling g^2 is large, only the first excited state $a = 1$ has an excitation energy $\epsilon = E_1 - E_{gd}$ that is exponentially smaller than all other $E_a - E_{gd}$. Thus, the corresponding $c_1(n)$ becomes exponentially large compared with all other $c_{a\neq 1}(n)$, in accordance with (1.21). Hence the iteration process (1.10) becomes rapidly convergent.

For a large class of problems in which $V(q)$ has high barriers and low valleys, there are often only a finite number of low-lying excited states.

$$a = 1,\ 2,\ \cdots,\ m \tag{1.22}$$

with excitation energies $\epsilon_a = E_a - E_{gd}$ comparable to each other, but exponentially smaller than those of $a > m$ states. By maintaining the orthogonality relations between these m low-lying excited states, the iteration process (1.10) can be readily generalized to such problems.

2. One Dimensional Problem

In one dimension, we replace $\{q_i\}$ by a single x. For simplicity, consider the special case

$$V(x) = V(-x). \tag{2.1}$$

Thus, the groundstate wave function $e^{-S(x)}$ is an even function of x and the first excited state $e^{-S(x)}\chi(x)$ an odd function. We assume that $e^{-S(x)}$ is already known, e.g. by following the method discussed in Refs.[1-4]. We further assume that the first excited state has an excitation energy

$$\epsilon << 1, \tag{2.2}$$

as would be the case if $V(x)$ is like the quartic potential (1.5) with large g. In one-dimension, (1.9) becomes

$$-\frac{1}{2}\frac{d}{dx}(e^{-2S}\frac{d\chi}{dx}) = \epsilon e^{-2S}\chi. \tag{2.3}$$

The corresponding series of iterative equations (1.10) for $n \geq 1$ is

$$-\frac{1}{2}\frac{d}{dx}(e^{-2S}\frac{d\chi_n}{dx}) = \epsilon_n e^{-2S}\chi_{n-1} \tag{2.4}$$

with χ_0 a properly chosen trial function. As in (1.13), in order to separate χ_n and ϵ_n from the ratio χ_n/ϵ_n we choose a fixed point x^0 and set

$$\chi_n(x^0) = \chi_0(x^0) \tag{2.5}$$

for all n.

In terms of the electrostatic analog (1.14)-(1.16), write

$$\kappa = e^{-2S}, \qquad \sigma_n = \epsilon_n e^{-2S}\chi_{n-1}$$

$$E_n = -\frac{1}{2}\chi_n' \quad \text{and} \quad D_n = \kappa E_n. \tag{2.6}$$

with $'$ denoting d/dx. Thus, (1.17) and (1.18) become

$$D_n'(x) = \sigma_n(x) \tag{2.7}$$

$$D_n(\pm\infty) = 0 \text{ and } \sigma_n(\pm\infty) = 0. \tag{2.8}$$

From (2.7) and (2.8), we have

$$D_n(x) = -\epsilon_n \int_x^\infty e^{-2S(z)}\chi_{n-1}(z)dz, \tag{2.9}$$

and therefore

$$E_n(x) = e^{2S(x)}D_n(x) \tag{2.10}$$

can also be readily expressed in terms of χ_{n-1}. Since $\chi_n(x)$ is odd in x, we need only to consider $x \geq 0$. From (2.6) and (2.10), we find

$$\chi_n(x) = 2\epsilon_n \int_0^x e^{2S(y)}dy \int_y^\infty e^{-2S(z)}\chi_{n-1}(z)dz. \tag{2.11}$$

Since $e^{-S(x)}$ is the groundstate, it has no zero at finite x. Thus, the factor $e^{2S(y)}$ in the y-integration of (2.11) is always finite. This is an important fact that enables us to extend the effectiveness of the iterative procedures of Refs.[1-5] for the groundstate to the low-lying excited state.

3. An Analytically Soluble Example

As an analytically soluble example, we consider the following simple one dimensional example

$$V(x) = \lambda\delta(x) + \begin{cases} 0 \ , & |x| < 1 \\ \infty \ , & |x| > 1. \end{cases} \tag{3.1}$$

The unnormalized groundstate solution is

$$e^{-S(x)} = \begin{cases} \sin p(1-x) & & 0 < x < 1 \\ 0 & \text{for} & |x| > 1 \\ \sin p(1+x) & & -1 < x < 0 \end{cases} \tag{3.2}$$

with

$$p \equiv \pi - \delta$$

and (3.3)

$$\lambda = -p\cot p = (\pi - \delta)\cot\delta.$$

For very large λ, p is very close to π, so

$$\delta \ll 1. \tag{3.4}$$

The exact lowest excited state is, for $|x| < 1$

$$e^{-S}\chi = \sin \pi x \tag{3.5}$$

with the excitation energy

$$\epsilon = \frac{1}{2}(\pi^2 - p^2) = \pi\delta - \frac{1}{2}\delta^2 \ll 1, \tag{3.6}$$

and for $x \geq 0$, χ is given by

$$\chi(x) = \frac{\sin \pi x}{\sin p(1-x)}. \tag{3.7}$$

In order to test the effectiveness of the iterative solution (2.11) and the supplementary condition (2.5), we shall start from the groundstate solution (3.2) and a trial function

$$\chi_0 = x. \tag{3.8}$$

Since (2.11) yields only the ratio $\chi_n(x)/\epsilon_n$, we follow (2.5) by choosing

$$x^0 = 1 \tag{3.9}$$

and therefore

$$\chi_n(1) = \chi_0(1) = 1. \tag{3.10}$$

It is clear that the trial function

$$e^{-S}\chi_0 = x \sin p(1-x) \tag{3.11}$$

is <u>not</u> a very good guess of the first excited state (3.5), nor does (3.8) resembles (3.7), except that at $x = 0$, $\chi_0(0) = \chi(0) = 0$. Nevertheless, we shall show that the iterative solution (2.11) with the supplementary condition (3.10) does lead to a rapidly convergent sequence.

Substituting (3.2) and (3.8) into (2.11), we find, for $x \geq 0$,

$$[\frac{4p}{2\epsilon_1} \sin p]\chi_1 e^{-S} = \sin px - (\sin p)[\frac{x}{p} \sin p(1-x) + x^2 \cos p(1-x)]. \tag{3.12}$$

The supplementary condition (3.10) leads to

$$\epsilon_1 = \frac{2p^2}{1 - p\cot p}. \tag{3.13}$$

For $\delta = \pi - p$ small, (3.13) gives

$$\epsilon_1 = 2\pi\delta - 4\delta^2 + 2(\frac{1}{\pi} + \frac{\pi}{3})\delta^3 - 2\delta^4 + O(\delta^5) \tag{3.14}$$

whereas the exact ϵ is given by (3.6) with $\epsilon_1 \cong 2\epsilon$. However, on second and third iterations, we find

$$\epsilon_2 = \pi\delta + (\frac{1}{\pi} - \frac{\pi}{3})\delta^3 + (\frac{1}{3} - \frac{2}{\pi^2})\delta^4 + O(\delta^5) \tag{3.15}$$

$$\epsilon_3 = \pi\delta - \frac{1}{2}\,\delta^2 + \frac{-6 + \pi^2}{12\pi}\,\delta^3 - \frac{15}{8\pi^2}\,\delta^4 + O(\delta^5). \tag{3.16}$$

Comparing to the exact value, the second order solution ϵ_2 gives the correct $\pi\delta$ and the third order ϵ_3 gives the correct first two terms: $\pi\delta - \frac{1}{2}\,\delta^2$.

For $\delta = 0.1$, (3.14)-(3.16) yield

$$\epsilon_1 = 0.59086, \quad \epsilon_2 = 0.31348, \quad \epsilon_3 = 0.30924 \tag{3.17}$$

which can be compared with the exact solution

$$\epsilon = 0.30916.$$

The $\chi_n(x)$ for $n = 0,\ 1,\ 2,\ 3$ are plotted in Fig.1, together with the exact solution $\chi(x)$. In fact, χ_2, χ_3 and χ are on the same curve. This shows the rapid convergence of the iterative process.

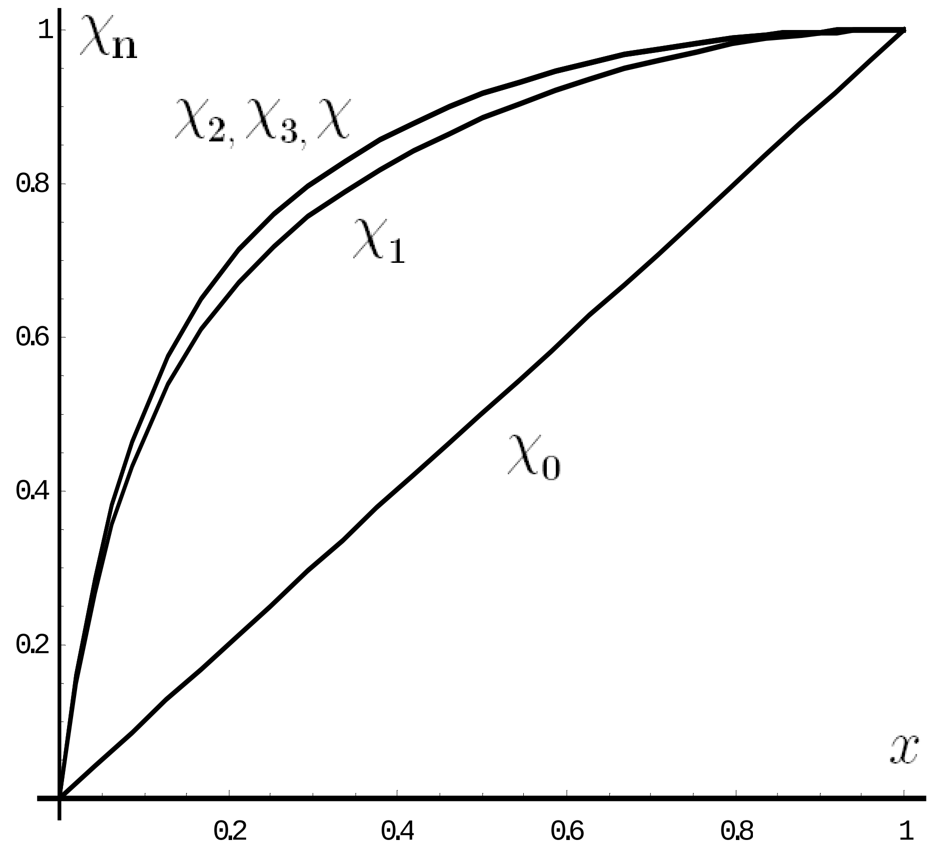

Fig.1 χ and χ_n for $n = 0,\ 1,\ 2,\ 3$ for the soluble problem (Section 3).

4. One-dimensional Quartic Potential

Consider the one-dimensional quartic potential

$$V = \frac{g^2}{2}(x^2-1)^2 \tag{4.1}$$

Assume that the groundstate wave function e^{-S} has been obtained by using the method described in our recent paper[5]. The first excited state $e^{-S}\chi$ satisfies (2.3) and the corresponding n^{th} order iterative solution is $e^{-S}\chi_n$, with χ_n given by (2.11). When $n=0$, we choose the trial function χ_0 to be an odd function, with

$$\chi_0(-x) = -\chi_0(x)$$

and for x positive

$$\chi_0(x) = \begin{cases} x(2-x) & \text{for} \quad 0<x<1 \\ 1 & \text{for} \quad x>1 \end{cases} \tag{4.2}$$

As in (2.5) and (3.9)-(3.10), we choose $x^0=1$ and set

$$\chi_n(1) = \chi_0(1) = 1. \tag{4.3}$$

In the following, we also set

$$g = 3. \tag{4.4}$$

Using the iteration method of Refs.[1,5], we find the groundstate energy to be

$$E_{gd} = 2.48291. \tag{4.5}$$

The lowest excitation energy ϵ_n for the first four iterations ($n = 1,\ 2,\ 3,\ 4$) based on (2.11) and (4.3) are

$$\epsilon_1 = 0.41776,\ \epsilon_2 = 0.41367,$$

$$\epsilon_3 = 0.413568,\ \epsilon_4 = 0.413568. \tag{4.6}$$

Thus, with three iterations, ϵ_3 is already accurate to seven significant figures. The corresponding wave functions χ_n are plotted in Figure 2. The groundstate e^{-S} and the first excited state $e^{-S}\chi$ are given in Figure 3. To the same seven significant figures the eigenvalue for the first excited state can be expressed as $E_{odd} = E_{gd} + \epsilon_4$.

To test the sensitivity to the choice x^0 we set, instead of (4.3), $x^0 = 1/2$ and require

$$\chi_n(\frac{1}{2}) = \chi_0(\frac{1}{2}). \qquad (4.7)$$

The corresponding excitation energies ϵ_n of the lowest excited state for the first 4 iterations are, in place of (4.6),

$$\epsilon_1 = 0.41363, \ \epsilon_2 = 0.41358$$

$$\epsilon_3 = 0.413569, \ \epsilon_4 = 0.413568. \qquad (4.8)$$

Alt
aft
me

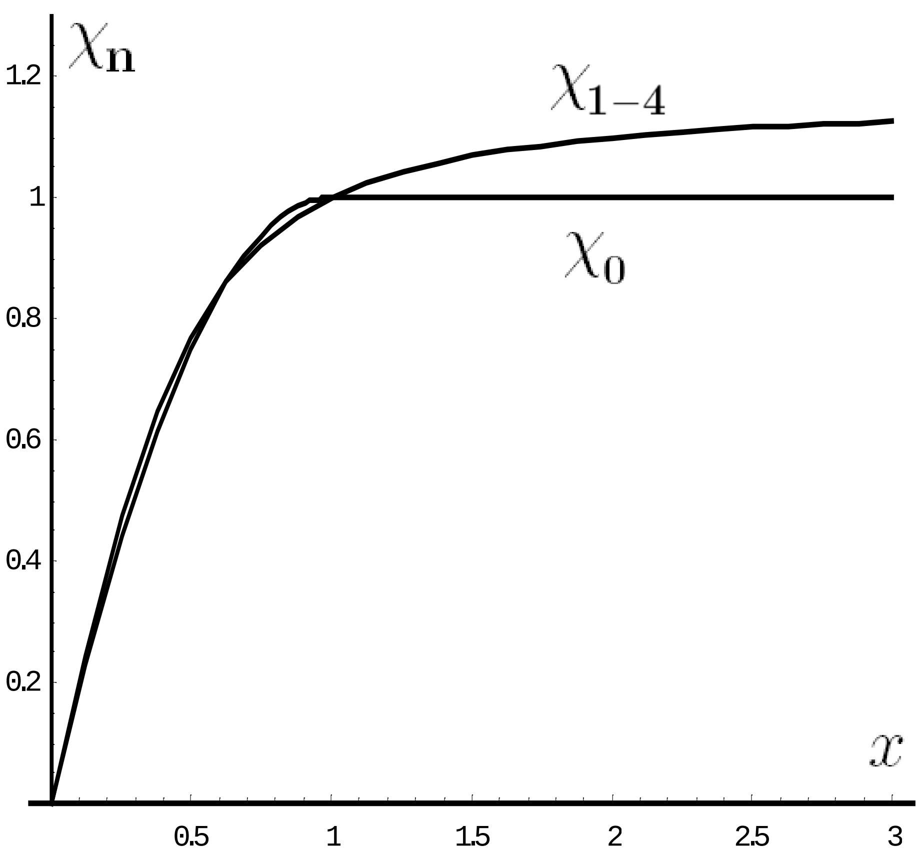

Fig.2 χ_n for $n = 0,\ 1,\ 2,\ 3,\ 4$ for the quartic potential (4.1) with $g = 3$.

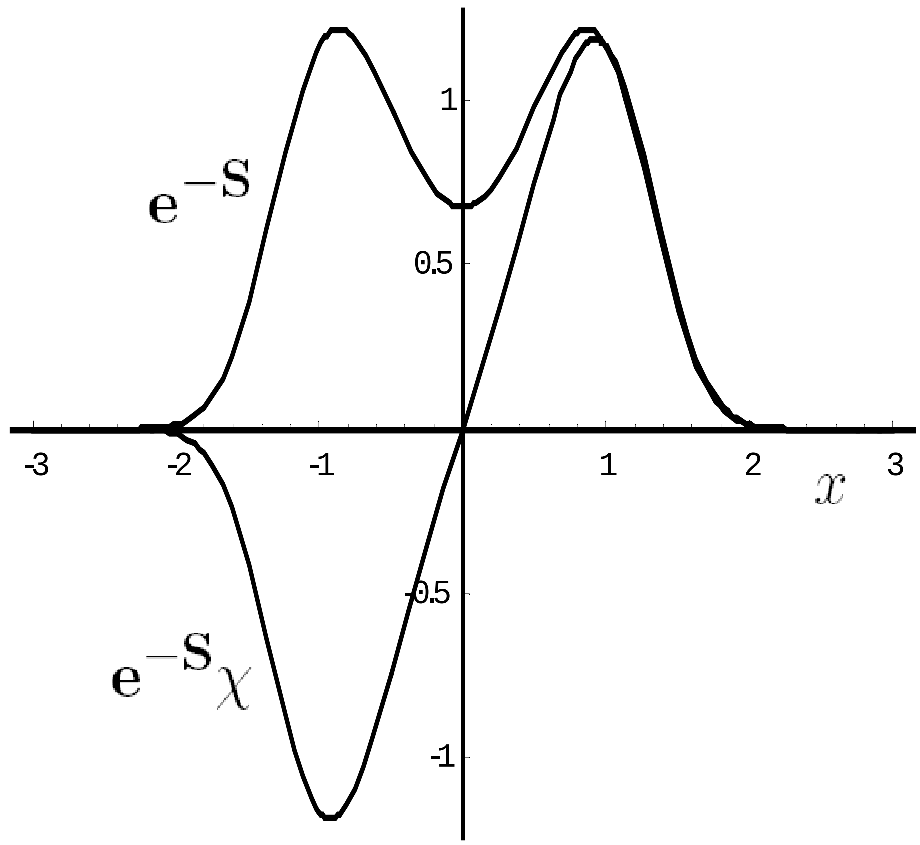

Fig.3 The groundstate wave function e^{-S} and the first excited state wave function $e^{-S}\chi$ for the quartic potential (4.1) with $g = 3$.

Appendix

In our earlier work[6] an asymptotic expansion of the average $E = \frac{1}{2}(E_{gd} + E_{odd})$ and that of the difference $\Delta = \frac{1}{2}\ \epsilon$ were obtained. To compare our present results with these asymptotic expansions, we take a larger coupling $g = 8$. This enables us to use the asymptotic expansion up to order $1/g^3$ for the wave function $\phi_\pm$ of Ref.[6]. We find

$$E_{asymp} = 7.728854\ . \tag{A.1}$$

Using the expressions

$$\Delta = \frac{\lambda}{2}\ \frac{1}{\int\limits_0^\infty \phi_+^2(x)dx} \tag{A.2}$$

and

$$\lambda = \phi'_+\phi_- - \phi_+\phi'_- \tag{A.3}$$

of Ref.[6], we obtain

$$\epsilon_{asymp} = 2\Delta_{asymp} = 0.003027. \tag{A.4}$$

For $g = 8$, the iterative method of Ref.[5] gives

$$E_{gd} = 7.727340. \tag{A.5}$$

The corresponding n^{th} order iterative excitation energy ϵ_n of Sec. 4 for $n = 1 - 4$ are

$$\begin{aligned} \epsilon_1 = 0.00310125,\ \epsilon_2 = 0.00301796 \\ \epsilon_3 = 0.003017947,\ \epsilon_4 = 0.003017947. \end{aligned} \tag{A.6}$$

Keeping the accuracy to seven significant figures, we find

$$E = E_{gd} + \frac{1}{2}\ \epsilon = 7.728849 \tag{A.7}$$

and

$$\epsilon = 0.003018. \tag{A.8}$$

Thus, the asymptotic values E_{asymp} and ϵ_{asymp} of (A.1) and (A.4) compare favorably well with E and ϵ of (A.7) and (A.8). However, inclusions of still higher

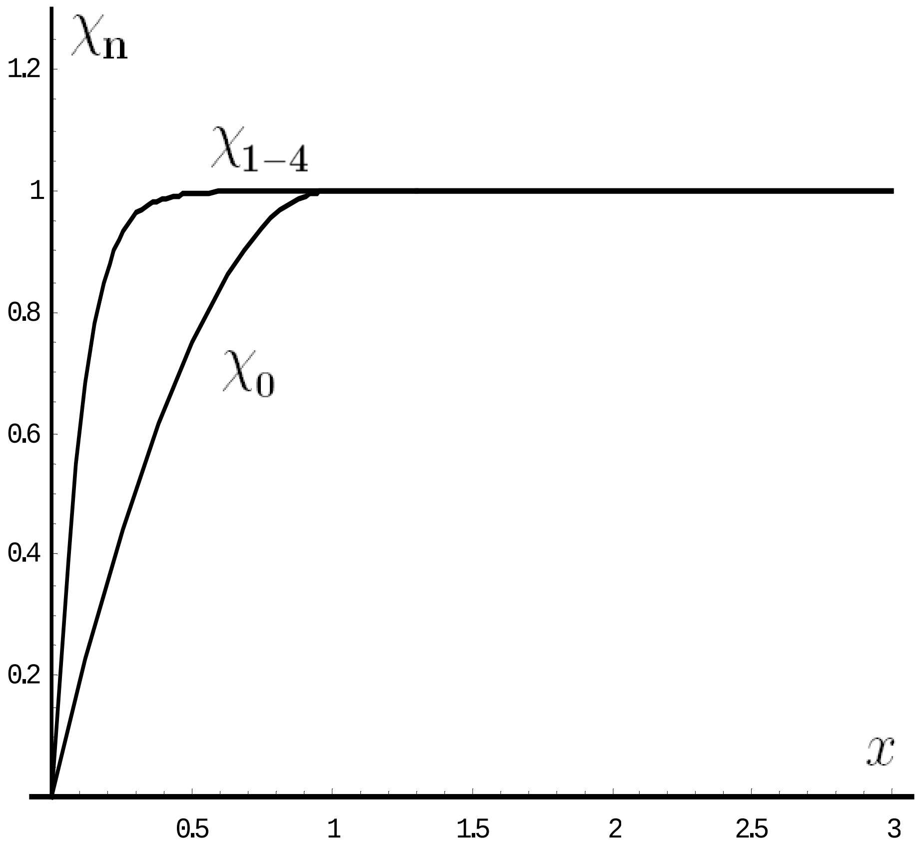

Fig.4 χ_n for $n = 0,\ 1,\ 2,\ 3,\ 4$ for the quartic potential (4.1) with $g = 8$.

and higher order terms in the asymptotic expansion would lead to divergent results for E_{asymp} and ϵ_{asymp}.

The wave functions $\chi_n(x)$ for $g = 8$ are plotted in Fig. 4. As we can see, the deviation of the $\chi_n(x)$ from 1 happens only at small x.

References

[1] R. Friedberg, T. D. Lee, W. Q. Zhao and A. Cimenser, Ann. Phys. 294(2001)67
[2] R. Friedberg and T. D. Lee, Ann. Phys. 308(2003)263
[3] R. Friedberg and T. D. Lee, Ann. Phys. 316(2005)44
[4] T. D. Lee, J. of Stat. Phys. 121(2005)1015
[5] R. Friedberg, T. D. Lee and W. Q. Zhao, Ann. Phys. in press, quant-ph/0510193
[6] R. Friedberg, T. D. Lee and W. Q. Zhao, IL Nuovo Cimento 112A(1999)1195